Critical Equalities for Potts Models

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Abstract

We apply a simple analytical criterion for locating critical temperatures to Potts models on square and triangular lattices. In the self-dual case, i. e. on the square lattice we reproduce known exact values of the critical temperature and derive the internal energy of the model at the critical point. For the Potts model on the triangular lattice we obtain very good numerical estimate of the critical temperature and also of the internal energy at the critical point.

1   Introduction

Critical temperature is known only for very few spin models like the two-dimensional Ising model, which is exactly soluble in $2d$, and Potts models where the critical temperature can be found by the duality relations [1-3]. In principle a position of the critical point can be obtained using one of many existing approximate techniques ranging from high and low temperature expansions to renormalization group methods. In this paper we employ a simple method based on the moments of the transfer matrix [4]. Let $\mathcal{T}$ be the transfer matrix for a d-dimensional spin system with linear size L and let $\beta = 1/k_B T$. One defines a characteristic function of rank n

$$\rho_n(\beta) = \lim_{L \to \infty} \left(\frac{(Tr\mathcal{T})^n}{Tr\mathcal{T}^n} \right)^{\frac{1}{L^{d-1}}}.$$ (1)

As was conjectured in [4] the maximum of ρ_n should occur at the critical point

$$\beta_{max} = \beta_{crit}.$$ (2)

The existing results suggest that the validity of the method is related to the dual properties of the system. It was checked directly for the Ising and Potts models with low q values on the square lattice that the criterion reproduces exact values of the critical temperature. It can be made exact also for the isotropic Ashkin-Teller model, for which the duality transformation involves three couplings. However, in this case the definition of the characteristic function should be modified [5,6]. On the other hand, for the two-layer Ising model, which is not self-dual, the criterion still gives surprisingly good numerical estimate of the critical temperature [7]. Therefore it is very tempting to perform further investigations of the method to test its applicability in different situations. This is a part of our programme whose final goal is an exact criterion for not self-dual systems.

In this paper we test the proposal (Eq. (2)) for the two-dimensional Potts model. Contrary to the previous mainly numerical work [4] our discussion is based on the explicit analytical expression for the function ρ_2 for arbitrary q. We also check some consequences arising from the criterion in the limiting case $n \to \infty$. These are interesting equalities relating internal energies of one and two dimensional systems. The calculation of ρ_2 is given in Section 2 and the equalities mentioned above are derived in Section 3. Appendix contains some technical details.

2   The ρ_2 function

The partition function of n coupled chains is related to the matrix T_n, which propagates horizontally n spins

$$Z_n = Tr\mathcal{T}^n = Tr(T_n)^L,$$ (3)

where L is the linear extension of the system as in the formula (1). The construction of the matrix T_n is shown, for $n = 2$, in Fig. 1 where periodic boundary conditions

are assumed in vertical direction. Since in the thermodynamic limit ($L \to \infty$) only the largest eigenvalue, $t_{n,max}$, of the matrix T_n dominates, we obtain for ρ_n the expression

$$\rho_n(\beta) = \frac{t_{1,max}^n}{t_{n,max}}, \tag{4}$$

which is very convenient for analytical calculations.

For the Potts model the matrices T_1 and T_2 have a simple form and it is relatively easy to find analytical expressions for the largest eigenvalues. This is done in the Appendix where the formulas for the ρ_2 function are given for square and triangular lattices. The functions $\rho_2(x)$, where $x = e^\beta$, for the Potts model on the square lattice are shown in Fig. 2. For arbitrary q they have the same characteristic shape with the maximum, whose height and position depend on q. The position of the maximum is located at $x = 1 + \sqrt{q}$ which agrees with the standard values obtained by duality of the six vertex model [1,3]. Indeed at this point the Potts model undergoes the second order transition for $q \leq 4$ and first order for $q > 4$.

The triangular lattice is not self-dual but it is dual to the honeycomb lattice. The exact critical temperature still can be found from some properties of ice-type models and it is given as a root of the cubic equation [1,3]

$$x^3 - 3x - q + 2 = 0. \tag{5}$$

The results for this case are summarized in Tab. 1, where we compare the critical values and the position of the maximum of ρ_2. The criterion still gives a good estimation of the critical temperature. In particular for $q = 2$ it is exact, which is related to the existence of the star-triangle relation which provides a certain kind of duality transformation.

3   Critical equalities

By taking the logarithm of (Eq. 1) and by differentiating it with respect to x one obtains the condition for the internal energies

$$u_1(x_{max}) = u_n(x_{max}), \tag{6}$$

where u_1 (u_n) denotes the density of the internal energy for a spin chain (n coupled spin chains). In the limit ($n \to \infty$) we conclude that at the critical point the energy density of the $2d$ system equals to the energy density of a single chain. This allows us to use standard expressions for the internal energy in Potts models to check validity of our criterion also in this limiting situation.

Let us first consider the square lattice. The internal energy of a chain per one spin is:

$$u_1 = \frac{2x + q - 1}{x + q - 1}. \tag{7}$$

3

Evaluating this at the critical point $x_{crit} = 1 + \sqrt{q}$ we obtain, in agreement with known results [1,3], namely that the energy of the $2d$ system is:

$$u_{crit} = 1 + \frac{1}{\sqrt{q}}. \tag{8}$$

For $q > 4$ when the system undergoes the first order phase transition the internal energy at the critical point is discontinuous. To fix this ambiguity one usualy defines the energy as a mean of the high and low temperature phase, and so should be interpreted our results.

In the last three rows of Tab. 1 we compare the predictions for numerical values of internal energies for the Potts system on the triangular lattice. $E(T_c)$ and L are results for the internal energy and latent heat respectively taken from Ref. [3]. $E(T_{max})$ is the energy of a single chain evaluated at the maximum point. The method still gives good numerical estimation of the internal energy. For the first order phase transition it fits nicely between energy of the high and low temperature phase.

The critical equalities are simple mathematical consequences of the maximum rule but their physical origin is unclear. One can say that at the critical point when the correlation length ξ diverges the interaction of a single chain with the rest of the $2d$ system can be simplified to the interaction of spins in a single chain with periodic boundary conditions. This would also mean that characteristic function should contain information about correlations in the system. Thus it should be possible to obtain other characteristics of the transition, for example to distinguish the order of the transition and to find the critical exponents. One can may be improve the method by combining it with the renormalization group techniques. It would also be tempting to look for signals of the order of transition containing in the function ρ_n. For the Potts model shape of ρ_2 exhibits rather slow crossover as a function of q and for the moment it is not clear weather one can see any particular change at $q = 5$.

Acknowledgements

4   Appendix

In this Appendix we derive analytical formulas for the ρ_2 function of the $2d$ Potts model. The energy of the q state Potts model is given by

$$E(s) = - \sum_{\langle i,j \rangle} \delta_{s_i, s_j}, \tag{9}$$

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where the sum runs over nearest neighbours sites labeled by i, j and the spin variables s are assumed to take q distinct values. The transfer matrices can be specified by their elements between spin states. For the square lattice they are:

$$
\begin{aligned}
\langle s|T_1|s'\rangle &= \exp\beta(\delta_{s,s'}+1), \\
\langle s_1 s_2|T_2|s_1' s_2'\rangle &= \exp\beta(\delta_{s_1,s_2}+\delta_{s_1,s_1'}+\delta_{s_2 s_2'}+\delta_{s_1' s_2'}).
\end{aligned}
\tag{10}
$$

It can be readily verified that $t_{1max} = x(x+q-1)$. The largest eigenvalue of the matrix T_2 can be obtained noting the special structure of the Potts interaction. To make it more evident we introduce an index $n = 0,\ldots,q^2-1$, which enumerates successive rows (columns) of the matrix. n can be represented as a two digit number in base q. With each digit we associate a spin variable. Let us now construct the equation for the eigenvalues. The 0-th, $(q+1)$-th,...,(q^2-1)-th row of the resulting determinant we multiply by some constant, say A. At the end we add all the rows to the last one. It is easy to notice that we generically obtain two expressions in the last row: in the 0-th, $(q+1)$-th,...,(q^2-1)-th column w_1 and in the other columns w_2. This is because the Potts interaction depends on whether two spins are equal or different. Detailed form of w_1 and w_2 can be obtained from some combinatorical considerations

$$
w_1 = A(x^4 - \lambda + (q-1)x^2) + (q-2)(q-1)x + 2(q-1)x^2, \tag{11}
$$
$$
w_2 = A(2x^2 + (q-2)x) + x^2 - \lambda + 2(q-2)x + q^2 - 3q + 3. \tag{12}
$$

If $w_1 = w_2 = 0$ one obtains a quadratic equation for a certain eigenvalue. We choose the larger root of this equation

$$
\lambda_1(x) = \frac{1}{2}(Q_2(x) + \sqrt{Q_3(x)}), \tag{13}
$$

where Q_2 and Q_3 are polynomials given below. The other eigenvalues $\lambda_i(x)$ $i = 2,\ldots,q^2$ can be considered as continuous functions of x. Moreover $\lambda_1(1) = q^2$, $\lambda_i(1) = 0$. By the Perron's theorem [8], $\lambda_1(x) \neq \lambda_i(x)$ since the elements of T_2 are positive. Thus $\lambda_1(x)$ must remain the largest eigenvalue in the whole interval $(1, \infty)$.

Collecting our results together we finally obtain:

$$
\rho_2(\beta) = \frac{Q_1(x)}{Q_2(x) + \sqrt{Q_3(x)}}, \tag{14}
$$

where

$$
\begin{aligned}
Q_1(x) &= 2x^2(x+q-1)^2, \tag{15} \\
Q_2(x) &= x^4 + qx^2 + (2q-4)x + q^2 - 3q + 3, \tag{16} \\
Q_3(x) &= x^8 + (2q-4)x^6 + (8-4q)x^5 + (-q^2 + 18q - 18)x^4 \\
&\quad + (12q^2 - 32q + 16)x^3 + (2q^3 - 6q^2 - 2q + 12)x^2 \\
&\quad + (4q^3 - 20q^2 + 36q - 24)x + (q^2 - 3q + 3)^2. \tag{17}
\end{aligned}
$$

The method described above applies also to the transfer matrices of the Potts model on the triangular lattice

$$
\begin{aligned}
\langle s|T_1 s\rangle &= \exp \beta(2\delta_{ss'} + 1) \\
\langle s_1 s_2|T_2|s_1' s_2'\rangle &= \exp \beta(\delta_{s_1,s_2} + \delta_{s_1,s_1'} + \delta_{s_2 s_2'} + \delta_{s_1' s_2'} + \delta_{s_1 s_2'} + \delta_{s_2 s_1'}).
\end{aligned} \tag{18}
$$

The final result has the same form as (14) with

$$
\begin{aligned}
Q_1(x) &= 2x^2(x^2 + q - 1)^2, \tag{19} \\
Q_2(x) &= x^6 + x^2(q+1) + x(4q - 8) + q^2 - 5q + 6, \tag{20} \\
Q_3(x) &= x^{12} + (2q - 6)x^8 + (-8q + 16)x^7 + \\
&\quad (-2q^2 + 26q - 28)x^6 + (17q^2 - 54q + 41)x^4 \\
&\quad + (-8q^2 + 40q - 48)x^3 + (2q^3 + 12q^2 - 74q + 84)x^2 \\
&\quad + (8q^3 - 56q^2 + 128q - 96)x \\
&\quad q^4 - 10q^3 + 37q^2 - 60q + 36. \tag{21}
\end{aligned}
$$

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q	2	3	4	5	6	7	8	...100
$e^{\beta_{cr}}$	$\sqrt{3}$	1.8794	2	2.1038	2.1958	2.2790	2.3553	4.8272
$e^{\beta_{max}}$	$\sqrt{3}$	1.8757	1.9930	2.0938	2.1893	2.2635	2.3373	4.7266
$E(T_c)$	0.8333	0.7603	0.7131	0.6881	0.6669	0.6506	0.6377	$\star$
$L(q)$	0	0	0	0.0310	0.1172	0.2042	0.2795	$\star$
$E(T_{max})$	0.8333	0.7584	0.7026	0.6819	0.6596	0.6404	0.6256	0.4561

Table 1: Comparison of the results taken from Ref. [3] and the values obtained from the maximum criterion for the 2d Potts model on the triangular lattice.
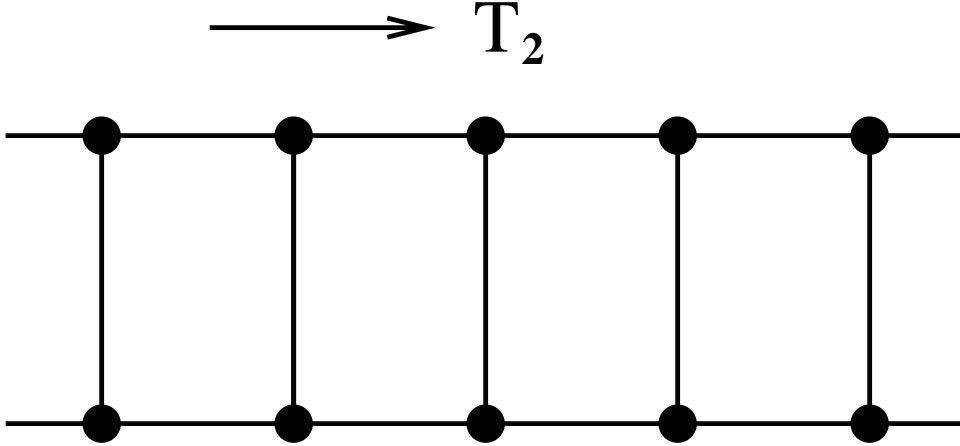

Figure 1: Construction of the transfer matrix T_2 for the two-dimensional Potts model on the square lattice. Periodic boundary conditions are assumed in vertical direction.
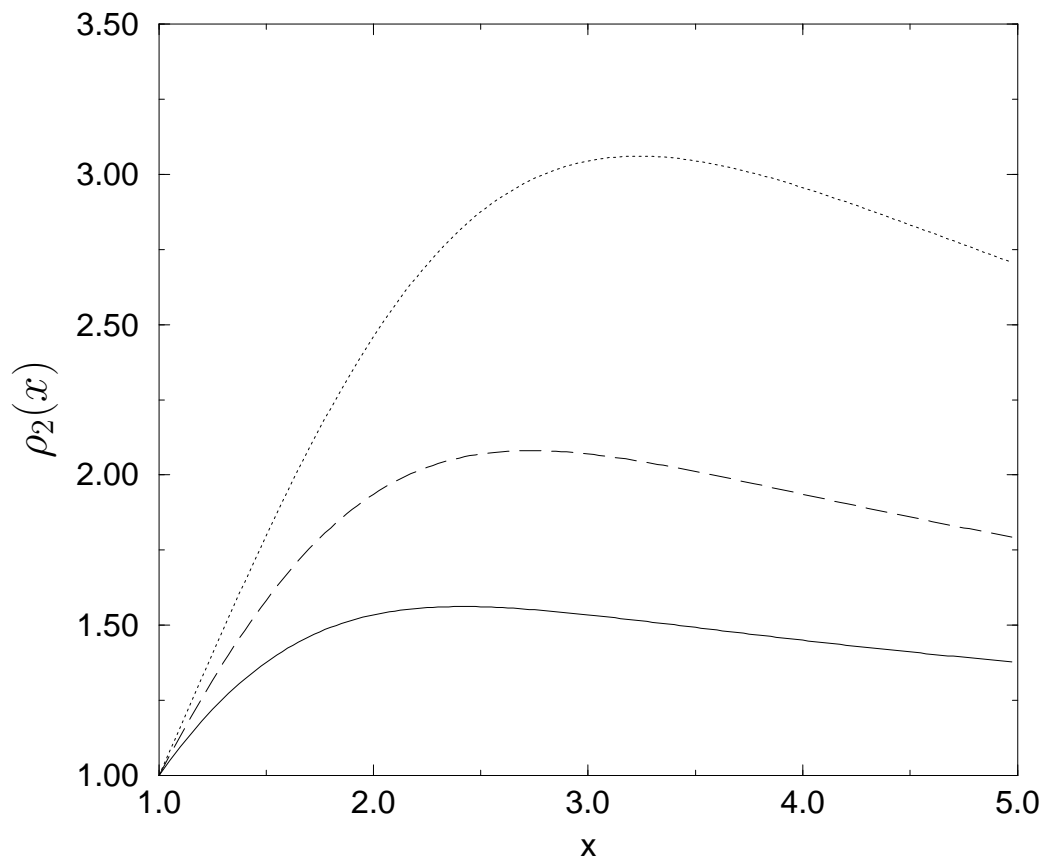
Figure 2: Functions ρ_2 for the Potts model on the square lattice. Three lines are shown for $q = 2$ (solid) , $q = 3$ (dashed) and $q = 5$ (dotted).